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Subdiffusive Reaction Front in the Enamel Caries Process

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Abstract

Starting with the equation describing subdiffusion associated with chemical reactions for one-static reactant, we show that the reaction front x_f evolves in time as $x_f \sim t^{\alpha/2}$ with $\alpha < 1$. The equation is applied to the carious lesion which is caused by the chemical reactions of diffusing acid molecules or pure hydrogen ions with static hydroxyapatite in the tooth enamel. Comparing our theoretical results with the already published experimental ones, we conclude that in some cases the transport process of the acids in the tooth enamel appears to be subdiffusive and should be described by the subdiffusion-reaction equation with the fractional time derivative.

Keywords: subdiffusion, reaction front, subdiffusion controlled reaction, carious lesion.

1. Introduction

The carious lesion starts in the tooth enamel which is composed of hydroxyapatite (HP). The caries is caused by hydrogen ions which react with the static HP. The organic acids are produced by metabolic activity of microorganisms in the dental plaque (see Fig.1). When a concentration of the acids and pH reach appropriate levels then the acids begin to diffuse inward enamel. The reaction causes dissolution of HA and thus the loss of mineral, which can reach about 70 per cent of its initial content. When the acids are transported in the dissociated form, one expects normal diffusion of the hydrogen ions inside the enamel due to the small size of the ions. An external structure of the enamel is rather complex but it can be treated as a porous medium. Therefore, the transport of large undissociated acid molecules can be subdiffusive because of strongly limited mobility of the molecules. This possibility is suggested by the experimental data concerning the time evolution of the caries limit inside the enamel. Connecting the caries limit with the reaction front (RF) x_f we show that for subdiffusion $x_f \sim t^{\alpha/2}$ with $\alpha<1$ whereas the case of $\alpha = 1$ corresponds to the normal diffusion transport [1].

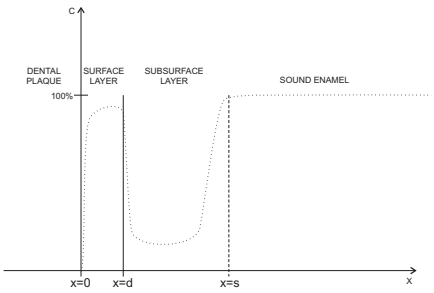

Fig.1. The schematic view of the tooth enamel. The dotted line represents the HA concentration

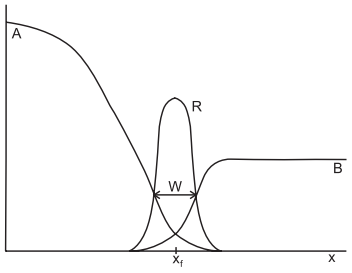

Fig.2. The reaction front.

2. The model

The subdiffusion-reaction equation includes the reaction term R which describes changes of the reactant concentration due to the chemical reactions. For the reaction $A+B\rightarrow C$(inert) the term is $R(x,t)=-kA(x,t)B(x,t)$ where k is the reaction rate while $A(x,t)$ and $B(x,t)$ denote the reactant concentrations. The reaction front (RF) is defined as a point where the reaction term reaches its maximum (see Fig.2). Taking into account that HA is static, the set of the subdiffusion-reaction equations are as follows

$$\frac{\partial^{\alpha} A(x,t)}{\partial t^{\alpha}} = D\frac{\partial^2 A(x,t)}{\partial x^2} - kA(x,t)B(x,t)\,,\quad \frac{\partial B(x,t)}{\partial t} = -kA(x,t)B(x,t)\,,$$

where $\partial^{\alpha}/\partial t^{\alpha}$ is the Riemann-Liouville fractional derivative. Solving the equations by means of the scaling method we find that for subdiffusion the RF evolves in time as $\sim t^{\alpha/2}$ with $\alpha<1$.

3. Conclusions

Comparing our theoretical results with the experimental ones (where α=2/3 was found), we conclude that in some cases the transport process of acids inside the enamel should be described by the subdiffusion-reaction equations with fractional time derivative. Our method allows to identify subdiffusion and to extract subdiffusion parameters form experimental data in a system with chemical reactions. Till now, such a method exists only for a system with pure subdiffusion [2].

References

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